bio-protocol Preprint

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Path CV driven metadynamics simulations with adaptive hills

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An abbreviated version of this protocol was published in eLIFE in Aug 2016

Mapping transiently formed and sparsely populated conformations on a complex energy landscape

DOI: 10.7554/eLife.17505

Detailed protocol

Dear Felipe
Thanks for your interest. We have deposited scripts and input files at:
https://github.com/KULL-Centre/papers/tree/master/2016/T4L-eLIFE-Wang-et-al
I hope you find them useful.
Kind regards
Kresten & Yong

How to cite:（Readers should cite both the Bio-protocol preprint and the original research article where this protocol was used）

1. Wang, Y. and Lindorff-Larsen, K. (2021). Path CV driven metadynamics simulations with adaptive hills. Bio-protocol Preprint. bio-protocol.org/prep891.
2. Wang, Y., Papaleo, E. and Lindorff-Larsen, K.(2016). Mapping transiently formed and sparsely populated conformations on a complex energy landscape. eLIFE. DOI: 10.7554/eLife.17505

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